

Terahertz Laboratory Spectroscopy of Iron Hydride Species FeH and FeH⁺

Completed Technology Project (2017 - 2020)



Project Introduction

Iron plays an important role in astrophysics. Having the one of the most stable binding energies of any element, it ranks 9th in overall cosmic abundance, with $\text{Fe}/\text{H} \sim 3 \times 10^{-5}$. It is sufficiently prevalent to be routinely used as a measure of metallicity in stars from its optical transitions. In the diffuse interstellar medium, iron appears to be depleted in the gas-phase by one to two orders of magnitude, based on ultraviolet absorption lines, suggesting that the element is incorporated into dust grains. The common occurrence of iron in meteorites and pre-solar grains bolsters this concept. On the other hand, type Ia supernovae, an major source of iron, show no evidence of dust grains in their ejecta. This result suggests that a large portion of iron remains in the gas phase. Some fraction of this gas-phase iron could be in molecular form. FeH and its corresponding ion, FeH⁺, are excellent molecular candidates, given the abundance of interstellar hydrogen. FeH itself has also been observed in the atmospheres of M-type stars and L-type brown dwarfs via electronic transitions in the near-infrared. However, probably the best technique for studying FeH and FeH⁺ in the general interstellar medium is via the pure rotational transitions of these species, which, because they are hydrides, only occur at sub-mm/THz/infrared wavelengths, and are often inaccessible by ground-based telescopes. Therefore, FeH and FeH⁺ are extremely good targets for sub-mm/THz NASA missions. The purpose of this proposal is to assemble a complete database of directly measured, highly accurate (1 part in 10⁷) rotational rest frequencies for FeH, its deuterium isotopologue FeD, and its ionic forms FeH⁺ and FeD⁺ in the frequency range 0.5 – 2 THz. Such a data set does not exist for either species, in part because spectroscopy of these molecules is not trivial. FeH has a highly perturbed, 4Δ_i ground electronic state, which precludes prediction of the THz rest frequencies from known infrared constants. There is no spectroscopic data of any sort for FeH⁺, and even its ground electronic state is uncertain, although theory suggests it is 5Δ_i. This project is well-matched to the PI's extensive experience in measuring and analyzing the spectra of iron-bearing molecules with exotic ground states, including those with perturbations (e.g. FeC (X3Δ_i), FeO (X5Δ_i), FeN (X2Δ_i), FeCN, (X4Δ_i), FeNC (X4Δ_i), FeO⁺ (X6Σ⁺)). Furthermore, the PI and her group already have preliminary measurements of a few sub-mm transitions of FeH and FeD, and thus the success of future work is highly probable. The technique to be employed for the measurements is sub-mm/THz direct absorption spectroscopy. Three working, proven spectrometers are available for this work, and the PI has already developed the unusual gas-phase synthetic techniques necessary to create these unstable species, and the spectroscopic expertise to analyze their open-shell electronic states. In addition, highly accurate quantum chemical calculations will be performed for FeH and FeH⁺ to provide additional molecular properties (dipole moments, line strengths), as well as assist in predicting the ground electronic state of the ion. Observations conducted in the past with Herschel Space Observatory and currently, SOFIA, have clearly demonstrated that simple hydride molecules such as NH, CH⁺, HF, SH⁺, HCl⁺, and OH⁺ are common



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Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

Lead Organization:

University of Arizona

Responsible Program:

Astrophysics Research and Analysis

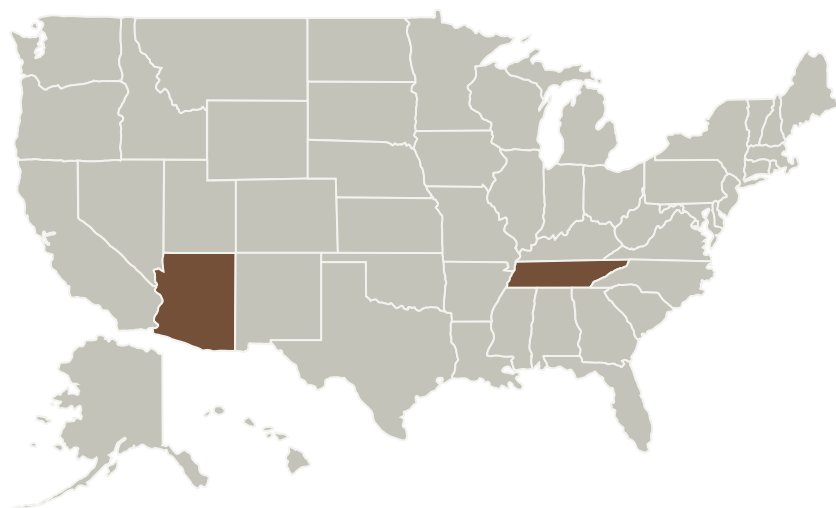
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constituents of many regions of the interstellar medium, even those with a rare element such as F or Cl. Moreover, other iron-containing molecules have been observed in circumstellar gas (FeCN in the outer envelope of the late-type carbon star IRC+10216) and possibly in dense molecular clouds (FeO in Sgr B2(M)). It would seem feasible that other Fe-bearing species would be present in interstellar gas. Hydrides have long been considered the building blocks of astrochemistry.

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
University of Arizona	Lead Organization	Academia Alaska Native and Native Hawaiian Serving Institutions (ANNH), Hispanic Serving Institutions (HSI)	Tucson, Arizona
University of Memphis	Supporting Organization	Academia Predominately Black Institutions (PBI)	Memphis, Tennessee

Project Management

Program Director:

Michael A Garcia

Program Manager:

Dominic J Benford

Principal Investigator:

Lucy M Ziurys

Co-Investigators:

Dewayne T Halfen
Nathan J Deyonker
Mary Gerrow

Technology Areas

Primary:

- TX08 Sensors and Instruments
 - └ TX08.3 In-Situ Instruments and Sensors
 - └ TX08.3.2 Atomic and Molecular Species Assessment

Target Destination

Outside the Solar System

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Primary U.S. Work Locations

Arizona

Tennessee